

# Semiclassical Theory of Bardeen-Cooper-Schrieffer Pairing-Gap Fluctuations

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Superfluidity and superconductivity are genuine many-body manifestations of quantum coherence. For finite-size systems the associated pairing gap fluctuates as a function of size or shape. We provide a theoretical description of the zero temperature pairing fluctuations in the weak-coupling BCS limit of mesoscopic systems characterized by order/chaos dynamics. The theory accurately describes experimental observations of nuclear superfluidity (regular system), predicts universal fluctuations of superconductivity in small chaotic metallic grains, and provides a global analysis in ultracold Fermi gases.

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A microscopic theory of superconductivity based on pairing was set up in 1957 by Bardeen, Cooper and Schrieffer [1]. These theoretical ideas were subsequently applied to finite systems by Bohr, Mottelson and Pines to describe ground-state superfluid properties of atomic nuclei [2]. Today pairing effects are central in a broad range of quantum systems, including neutron stars, metallic grains, atomic gases, nuclei, etc [3, 4, 5, 6]. As the system size diminishes, finite-size effects become important and lead to corrections with respect to the bulk homogeneous behavior. Of particular interest is the influence of the discreteness of the single-particle quantum energy levels. In connection with superconductivity, its importance was initially emphasized by P. W. Anderson [7], who pointed out that superconductivity in small metallic grains should disappear when the single-particle mean level spacing becomes of the order of the pairing gap. The validity of this criterion was qualitatively confirmed experimentally in the 90's [8]. Another consequence of the discreteness of the energy levels is the appearance of fluctuations as a parameter is varied. There is at least one clear experimental evidence of fluctuations of the pairing gap in superfluid systems, through the odd-even staggering of nuclear masses as a function of the mass number.

Our purpose here is to present, within a mean-field approximation, a theory of the pairing-gap fluctuations valid in the weak coupling BCS limit for arbitrary ballistic potentials. Our method is based on periodic orbit theory, which has been successful in describing mesoscopic fluctuations of thermodynamic and transport properties in many-body systems [9]. The results allow for a detailed calculation of the fluctuations in specific systems. In particular, they provide an accurate description of the pairing fluctuations in nuclei (cf Fig. 2). We also focus on statistical properties, which are shown, generically, to be non-universal. The analysis leads to a global and complete picture of the typical size of the fluctuations in terms of properties of the corresponding classical system, namely regular or chaotic dynamics.

Our starting point is the mean field BCS equation for

the pairing gap  $\Delta$  [1],

$$\frac{2}{G} = \int_{-L}^L \frac{\rho(\varepsilon)d\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}}, \quad (1)$$

where  $G$  fixes the strength of the pairing (seniority) interaction,  $\rho(\varepsilon)$  is the single-particle level density, and we have put the Fermi energy to zero. The energy cut off  $\pm L$  is given by the physical conditions, that are often related to the determination of the force strength  $G$ . Following semiclassical approaches, we divide the pairing gap as well as the single-particle density of states in a smooth part and a fluctuating part,  $\Delta = \bar{\Delta} + \tilde{\Delta}$  and  $\rho = \bar{\rho} + \tilde{\rho}$ , respectively. In the weak coupling limit  $\Delta \ll L$ , the smooth part of the gap is given by the well known solution  $\bar{\Delta} = 2L \exp(-1/\bar{\rho}G)$  (see Ref. [10] for regularization schemes). The fluctuating part of the density  $\tilde{\rho}$  can be expressed as [9]

$$\tilde{\rho}(\varepsilon) = 2 \sum_p \sum_{r=1}^{\infty} A_{p,r} \cos(rS_p/\hbar + \nu_{p,r}), \quad (2)$$

where the sum is over all primitive periodic orbits  $p$  (and their repetitions  $r$ ) of the classical underlying effective single-particle Hamiltonian. Each orbit is characterized by its action  $S_p$ , stability amplitude  $A_{p,r}$ , period  $\tau_p = \partial S_p / \partial \varepsilon$  and Maslov index  $\nu_{p,r}$  (all evaluated at energy  $\varepsilon$ ). Assuming  $\tilde{\Delta} \ll \bar{\Delta}$ , an equation for  $\tilde{\Delta}$  may be obtained by multiplying Eq. (1) by  $\Delta$ , replacing the single-particle level density by its semiclassical expression, and expanding up to lowest order in fluctuating properties. Assuming moreover  $\bar{\Delta} \ll L$  gives

$$\tilde{\Delta} = \frac{\bar{\Delta}}{\bar{\rho}} \sum_p \sum_{r=1}^{\infty} A_{p,r} Y(r\tau_p) \cos\left(\frac{rS_p}{\hbar} + \nu_{p,r}\right), \quad (3)$$

where

$$Y(\tau) = \int_{-\infty}^{\infty} d\varepsilon \frac{\cos(\tau\varepsilon/\hbar)}{\sqrt{\varepsilon^2 + \Delta^2}} = 2K_0(\tau/\tau_{\Delta}). \quad (4)$$

This equation, where all classical quantities involved are evaluated at Fermi energy, contains detailed information about the variations of the pairing gap. Note that  $\tilde{\Delta}$  only depends on  $G$  and  $L$  through  $\Delta$ .  $K_0(x)$  is the modified Bessel function of second kind. Through it, a new characteristic “pairing time” associated with the pairing gap is introduced,

$$\tau_\Delta = \frac{\hbar}{2\pi\tilde{\Delta}}. \quad (5)$$

Since  $K_0(x) \propto \exp(-x)/\sqrt{x}$  for  $x \gg 1$ , the Bessel function exponentially suppresses all contributions for times  $\tau \gg \tau_\Delta$  (making the sum convergent). The average part of the gap  $\tilde{\Delta}$  is thus playing, in this respect, a role very similar to the temperature in the general theory of mesoscopic fluctuations (cf Ref. [11]). In contrast,  $K_0(x) \propto -\log(x)$  for  $x \ll 1$ , and short orbits (compared to  $\tau_\Delta$ ) are logarithmically enhanced.

Since the value of the actions depend on the shape of the mean-field potential, Eq. (3) predicts, generically, fluctuations of the pairing gap as one varies, for instance, the particle number, or the shape of the system at fixed particle number. The fluctuations result from the interference between the different oscillatory terms that contribute to  $\tilde{\Delta}$ . The symmetries of the potential and the nature (integrable or chaotic) of the underlying classical motion are crucial to understand the interference pattern. When the motion is regular (integrable), continuous families of periodic orbits having the same action, amplitude, etc, exist. The coherent contribution to the sum (3) of these families of periodic orbits produces large fluctuations. In contrast, in the absence of regularity or symmetries, incoherent contributions of smaller amplitude coming from isolated unstable orbits are expected. Moreover, aside the dependence on the regular or chaotic nature of the single-particle motion, the presence or absence of universality in the statistical properties of the fluctuations will depend on the dominance of short or long periodic orbits.

We will make below an analysis of the predictions of Eq. (3) in the nuclear case, as the neutron number is varied. Before, and in order to avoid at this stage a detailed study of a particular system, we concentrate on a global analysis, namely the typical size or root mean square (RMS) of the BCS gap fluctuations in a generic mesoscopic system. The second moment of the fluctuations may be expressed from Eq. (3) as

$$\langle \tilde{\Delta}^2 \rangle = \frac{\tilde{\Delta}^2}{2\tau_H^2} \int_0^\infty d\tau Y^2(\tau) K(\tau), \quad (6)$$

where  $\tau_H = \hbar/\delta$  is Heisenberg time ( $\delta = \bar{\rho}^{-1}$  is the single-particle mean level spacing at Fermi energy), and  $K(\tau)$  is the spectral form factor, i.e. the Fourier transform of the two-point density-density correlation function [12].

The structure of the form factor  $K(\tau)$  is characterized by two different time scales. The first one, the smallest

of the system, is the period  $\tau_{\min}$  of the shortest periodic orbit. The form factor is zero for  $\tau \leq \tau_{\min}$ , and displays non-universal (system dependent) features at times  $\tau_{\min} \lesssim \tau \ll \tau_H$ . As  $\tau$  further increases, the function becomes universal, depending only on the regular or chaotic nature of the dynamics, and finally tends to  $\tau_H$  when  $\tau \gg \tau_H$ . The result of the integral (6) thus depends on the nature of the dynamics, and on the relative value of  $\tau_\Delta$  with respect to  $\tau_{\min}$  and  $\tau_H$ . According to Anderson criterion [7], superconductivity exists if  $\tilde{\Delta} > \delta$  (we are not interested here in the ultrasmall regime  $\tilde{\Delta} < \delta$  [13] where the BCS theory fails). Then,  $\tilde{\Delta} > \delta$  implies  $\tau_\Delta/\tau_H = \delta/2\pi\tilde{\Delta} \ll 1$ . Because the Bessel function  $K_0$  exponentially suppresses the amplitude for times  $\tau \gg \tau_\Delta$ , one can safely ignore the structure of the form factor for times of the order or bigger than  $\tau_H$ , and use the so called diagonal approximation of  $K(\tau)$  [12]. In the simplest approximation, all the non-universal system-specific features are taken into account only through  $\tau_{\min}$  [11], and one can write  $K(\tau) = 0$  for  $\tau < \tau_{\min}$  and, for  $\tau \geq \tau_{\min}$ ,  $K(\tau) = \tau_H$  for integrable systems and  $K(\tau) = 2\tau$  for chaotic ones with time reversal symmetry.

This finally gives the expressions for fluctuations of the pairing gap (normalized to the single-particle mean level spacing),  $\sigma = \sqrt{\langle \tilde{\Delta}^2 \rangle}/\delta$ , assuming regular dynamics [14],

$$\sigma_{\text{reg}}^2 = \frac{\pi}{4} \frac{\tilde{\Delta}}{\delta} F_0(D), \quad (7)$$

and assuming chaotic dynamics,

$$\sigma_{\text{ch}}^2 = \frac{1}{2\pi^2} F_1(D), \quad (8)$$

where  $F_n(D) = 1 - \int_0^D x^n K_0^2(x) dx / \int_0^\infty x^n K_0^2(x) dx$ . The argument

$$D = \frac{\tau_{\min}}{\tau_\Delta} = \frac{2\pi}{g} \frac{\tilde{\Delta}}{\delta} \quad (9)$$

is a system dependent quantity inversely proportional to the dimensionless conductance,  $g = \tau_H/\tau_{\min}$ , an intrinsic characteristic of the system independent of the pairing coupling.  $D$  can also be viewed as the system size divided by the coherence length of the Cooper pair,  $\xi_0 = \hbar v_F / (2\tilde{\Delta})$ , where  $v_F$  is Fermi velocity. Equations (7) and (8), which together with Eq. (3) are the main results of this study, show that the variance of the pairing gap is a function of its normalized mean part,  $\tilde{\Delta}/\delta$ , and of the dimensionless conductance,  $g$ , as shown in Fig. 1.

The monotonic function  $F_n(D)$  has the following limiting behaviors,  $F_n(D) \rightarrow 1$  as  $D \rightarrow 0$ , whereas  $F_n(D) \rightarrow 0$  exponentially fast for  $D \gg 1$ . Thus, in a system characterized by large  $g$ -value,  $D \rightarrow 0$ . In this case  $F_n(D) \rightarrow 1$ , all dynamical system specific properties disappear, and we obtain a “universal” (system independent) behavior

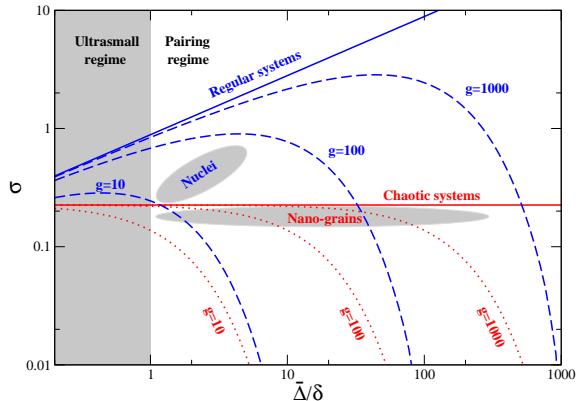


FIG. 1: Fluctuations of the pairing gap as a function of the mean value for mesoscopic systems (log-log scale; all quantities normalized with the single-particle mean spacing). The dashed (regular, in blue) and dotted (chaotic, in red) curves correspond to different values of the dimensionless conductance,  $g$ , and the limiting case of  $g \rightarrow \infty$  is shown by solid lines. The results are valid in the pairing regime  $\bar{\Delta}/\delta > 1$ . Applications to Nuclei and Nano-grains are marked out. Ultracold atomic gases may be controlled to appear in major parts of the figure.

of the gap fluctuations given by the prefactors in Eqs. (7) and (8), that correspond to a pure uncorrelated Poisson sequence and to a GOE random matrix spectrum, respectively (the latter,  $\sigma_{\text{ch}}^2 = 1/(2\pi^2)$ , was obtained previously in Ref. [13]). This situation is shown by the solid lines in Fig. 1: purely GOE fluctuations imply a constant amplitude of the normalized fluctuations of the pairing gap, whereas an increase with  $\bar{\Delta}/\delta$  is seen for systems with uncorrelated spectra. In contrast, in the generic case of systems characterized by finite values of  $g$ ,  $F_n$ , and therefore the pairing fluctuations, may significantly deviate from universality (cf Fig. 1). Thus, in general, pure statistical models (like GOE) do not provide an adequate description of the pairing fluctuations.

We shall now apply these results to different physical situations. Our first example is a system dominated by regular dynamics, namely ground states of atomic nuclei, which bring the best experimental data available at present on the superfluidity of finite Fermi systems. The ground-state superfluidity of atomic nuclei implies a mass difference between systems with an even and odd number of particles. The connection between the pairing gap and the mass differences is given by the three-point measure  $\Delta_3(M) = B(M) - [B(M+1) + B(M-1)]/2$ , where  $M$  is the odd neutron  $N$  or proton  $Z$  number. In the presence of other possible interactions, this quantity has been shown to be a very good measure of pairing correlations [15].  $\Delta_3$  is shown in Fig. 2 for neutrons. The average dependence of the neutron and proton gaps is well approximated, from experimental data, by

$$\bar{\Delta} = \frac{2.7}{A^{1/4}} \text{ MeV} , \quad (10)$$

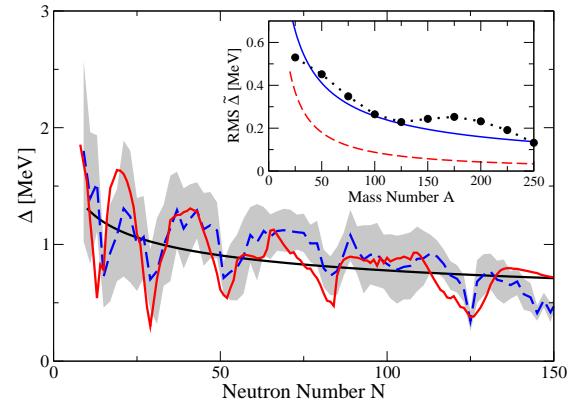


FIG. 2: Nuclear pairing gaps for neutrons. The blue dashed line shows average experimental gaps, and isotopic variation within one standard deviation is marked by the shaded area. Calculations from the cavity model are shown by the solid red line. Average behavior (Eq. (10)) is shown by solid black line. Inset: RMS of pairing gap fluctuations versus mass number  $A$ . The dots are experimental data for protons and neutrons. Solid and dashed lines are regular (Eq. (7)) and chaotic (Eq. (8)) predictions. Data from Ref. [24].

where  $A = N + Z$  is the total number of nucleons [16]. We notice a rather strong variation around the average value. The  $A$  dependence of the RMS of the experimental pairing fluctuations is shown in the inset of Fig. 2.

In order to evaluate the RMS of the pairing fluctuations from the theoretical expressions, Eqs. (7) and (8), we need the following estimates of nuclear properties (for one nucleon type): mean level spacing,  $\delta \approx 50/A$  MeV, and dimensionless conductance  $g \approx 1.6A^{2/3}$  [17]. This gives  $D \approx 0.21A^{1/12}$ , which ranges from 0.27 for  $A = 25$  to 0.33 for  $A = 250$ . Though these values clearly set atomic nuclei in the regime  $\tau_{\min}/\tau_{\Delta} < 1$  where pairing fluctuations are important, we are still far from  $D = \tau_{\min}/\tau_{\Delta} = 0$ , so that significant deviations from universality are expected. By inserting these estimates in Eqs. (7) and (8) the fluctuations are easily evaluated, assuming regular or chaotic dynamics. The resulting curves are compared to the experimental one in the inset of Fig. 2. Note, as expected [18], the good agreement between the regular dynamics and the experimental curve, either in the overall amplitude as well as in the  $A$ -dependence.

One may go beyond a statistical description, and use Eq. (3) to obtain a detailed description of the fluctuations. For that purpose, we assume for the nuclear mean field a simple hard-wall cavity potential. The shape of the cavity at a given number of nucleons is fixed by minimization of the energy against quadrupole, octupole and hexadecapole deformations. To simplify, we take  $N = Z$ . The periodic orbits of a spherical cavity are used in Eq. (3), with modulations factors that take into account deformations and inelastic scattering [19]. We set the average of  $\tilde{\Delta}$  to zero, as was done with the exper-

imental data (although of interest by itself, we will not consider its behavior here). In Fig. 2 we compare the theoretical result  $\bar{\Delta}(N)$  to the experimental value averaged over the different isotopes at a given  $N$ . The agreement is excellent; the theory describes all the main features observed in the experimental curve.

Our second example are the superconducting properties of nano-sized clean (ballistic) metallic grains [20], where we may expect the dynamics to be chaotic, see Ref. [4]. The existence of a superconducting gap was demonstrated in the regime  $\bar{\Delta} > \delta$  [8], whereas no gap was observed when  $\bar{\Delta} < \delta$  (the transition occurs around  $N \sim 5000$ , where  $N$  is the number of conduction electrons in the grain). The  $N$  dependence of the average gap  $\bar{\Delta}$  is poorly understood. We will adopt for grains the thin-film value  $\bar{\Delta} \approx 0.38 \times 10^{-3}$  eV [4]. The mean level spacing is  $\delta = (2E_F)/(3N) \approx 2.1/N$  eV, whereas  $g \approx 2.6N^{2/3}$ . Eq. (9) gives  $D \approx 4.4 \times 10^{-4}N^{1/3}$ , which ranges from 0.05 to 0.02 when  $N$  varies between  $10^3$  and  $10^5$ . This means that the variance will be close to its “universal” value obtained by setting  $F_1(D) = 1$  in Eq. (8), namely  $\sigma_{\text{ch}}^2 = 1/2\pi^2$ . Their typical range of variation is represented in Fig. 1.

In the case of chaotic dynamics, we don't have explicit experimental or numerical data to compare with. We can, alternatively, compute the fluctuations of the condensation energy, defined as the total energy difference between the paired and unpaired system. In the universal chaotic limit, our results are in good agreement with the numerical calculations of Sierra *et al.* [21], where they use Richardson's solution of the pairing problem and random matrix theory (GOE) for generating the single-particle spectrum.

Superfluidity in ultracold atomic gases is currently intensively studied, and provides our third example. The confinement potential can be externally controlled to create regular as well as chaotic dynamics, and the atom-atom interaction,  $a$ , can be tuned around the Feshbach resonance. Since both particle number and interaction strength are experimentally controlled parameters, the fluctuations may appear in major parts of Fig. 1. We estimate  $\delta = (2E_F)/(3N)$  and  $g = \frac{1}{2}(3N)^{2/3}$ ; in the dilute BCS region  $\bar{\Delta} = (2/e)^{7/3}E_F \exp(-\pi/2k_F|a|)$  [22], with  $k_F$  the Fermi wavevector, giving  $D = 2\pi(2/e)^{7/3}(3N)^{1/3} \exp(-\pi/2k_F|a|)$ . Recent experiments using Li<sup>6</sup> reach  $k_F|a| = 0.8$  [23], implying negligible fluctuations for typical values of  $N \sim 10^6$ . Reducing to  $k_F|a| = 0.2$  and  $N = 10^4$  yields for generic regular systems fluctuations that are on the same magnitude as the mean pairing gap,  $\sigma_{\text{reg}} \approx 0.5\bar{\Delta}/\delta$  [14].

To conclude, we have presented an explicit semiclassical theory for the pairing gap fluctuations. These are generically dominated by system specific features not included in purely statistical models. Different possible regimes, as well as the influence of order/chaos dynam-

ics, were investigated, in particular for the typical size of the fluctuations (Fig. 1). The present theory provides, for the first time, analytic predictions, valid for a wide range of physical situations; it also compares very favorably with available experimental data.

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